

# **Extraction and Semi-metric Analysis of Social and Biological Networks**

### Luis M. Rocha

Complex Systems Modeling
CCS3 - Modeling, Algorithms, and Informatics
Los Alamos National Laboratory, MS B256
Los Alamos, NM 87545
and
Center for Computational Biology
Instituto Gulbenkian de Ciência
Oeiras, Portugal



NASA's Goddard Space Flight Center Information Science & Technology (IS&T) Colloquium January 29, 2003



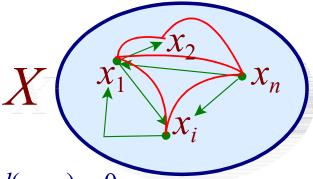
Luis Rocha 2002



# **Distances on Graphs**

Measured from associative "knowledge" graphs

d is a distance function on set X if it is a nonnegative, symmetric, real-valued function such that d(x, x) = 0 (Shore & Sawyer 1993)



 $d(x_i, x_i) = 0$   $d(x_i, x_j) = 1$ , if there is an edge  $d(x_i, x_k) = d(x_i, x_j) + .... + d(x_l, x_k) 1$ , if there is a path

Due to the symmetry requirement, distance functions yield non-directed distance graphs

$$d(x_1, x_2) \le d(x_1, x_3) + d(x_3, x_2)$$

**Metric**: the smallest distance between nodes is always the most direct path

 $X_{1} \underbrace{x_{2} w_{n2}}_{w_{1i}} x_{n}$ 

In real-valued weighted graphs, derived distance functions can be semi-metric

$$d(k_1, k_2) > d(k_1, k_3) + d(k_3, k_2)$$

Semi-metric

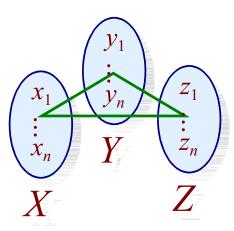
In graphs used to store "knowledge", what does it mean?

Luis Rocha 2002



# **Mathematical Background**

#### Relations



$$r(x_i, y_j, z_k) = 1$$

Represent the presence or absence of association, interaction or interconnectedness between the elements of two or more sets.

- a relation R between sets  $X_1, X_2, ..., X_n$  is a subset of the Cartesian product of these sets:  $R(X_1, X_2, ..., X_n) \subseteq X_1 \times X_2 \times ... \times X_n$ .
  - Traditional logical operations between sets can be used to modify relations

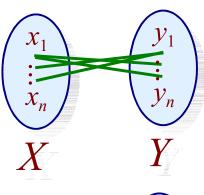
$$R(x_1, x_2, ..., x_n) = \begin{cases} 1 & \text{iff}(x_1, x_2, ..., x_n) \in R \\ 0 & \text{otherwise} \end{cases}$$

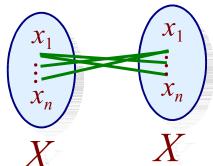
 $R(\mathbf{x}) \in [0,1], \quad \forall \mathbf{x} \in \mathbf{X}$  Fuzzy: Degree of Relation or association

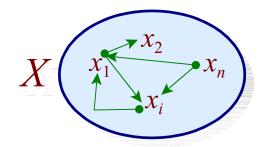
Luis Rocha 2002



### **Binary Relations**







- Binary fuzzy relations are a generalization of real functions
  - ► Two or more elements of Y may relate to an element of X
  - Easily represented by matrices of dimension n×m

- Graphs are binary relations defined on a single set: R(X, X).
  - Degrees of association between elements of the same set
  - ► If symmetric, *R* represents a non-directed graph

Luis Rocha 2002





## **Fuzzy Graphs**

#### **Properties**

#### Reflexive

- iff R(x, x) = 1 for all  $x \in X$ 
  - every element of X is maximally associated with itself
- Symmetric
  - iff R(x, y) = R(y, x) for all  $x, y \in X$ 
    - Matrices require only  $(n^2-n)/2$  elements to be defined
- (Max-Min) Transitive
  - iff  $R(x, z) \ge \max_{y \in X} \min[R(x, y), R(y, z)]$  for all  $x, z \in X$ 
    - For each indirect connection between x and z through some y, the weight of the connection is the smallest of each connection (x to y and y to z). Finally, the weight of the connection between x and z, is the largest of all indirect connections through all y (strongest path defined by weakest link)







### **Composition of Fuzzy Graphs**

Max-Min Composition:  $R \circ R = \max_{k} \min(r_{ik}, r_{kj}) = r'_{ij}$ 

where  $r_{ij}$  denotes  $R(x_i, x_j)$ 

The max-min (logical) composition of matrices is performed in the same way as the numerical counterpart, except that multiplication and summation are substituted by the *Min* (and) and *Max* (or) operations respectively.

- Transitive closure of a relation R(X, X)
  - ► The relation that is transitive, contains R(X, X), and whose elements have the smallest possible membership weights that still allow the first two requirements.
    - It yields a relation where all pairs of elements which were directly or indirectly related in the original relation, are now directly related
    - 1.  $R' = R \cup (R \circ R)$ ; 2. If  $R' \neq R$ , make R = R' and go back to step 1; 3. Stop:  $R_T = R'$

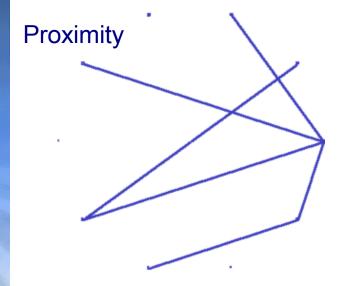


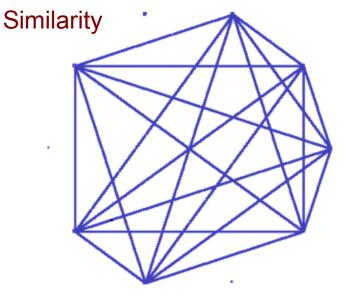


# **Similarity and Proximity Relations**

### Similarity Relation

- ► A reflexive, symmetric, and transitive binary fuzzy relation
  - Also known as an equivalence relation.
- Proximity Relation
  - A reflexive and symmetric binary fuzzy relation
    - Also known as a compatibility relation
    - The transitive closure of a proximity relation is a similarity relation.





Luis Rocha 2002





### Measuring "Knowledge" Associations

From Document Relations

- Document × Document
  - Co-Citation or Hyperlink structure
- Document × Keyterms
  - ► Keyterm Co-Occurrence
- Document/Dataset × Gene Expression
  - ► Gene Co-Occurrence or Co-Expression
- Document × Author
  - Co-Authorship (Collaboration Network)

Given a binary relation R between sets X and Y we extract two proximity relations:  $XYP(x_i, x_j)$  is the probability that both  $x_i$  and  $x_j$  are related in R to the same element  $y \in Y$ . Conversely,  $YXP(y_i, y_j)$  is the probability that both  $y_i$  and  $y_j$  are related in R to the same element  $x \in X$ .

$$XYP(x_{i}, x_{j}) = \frac{\sum_{k=1}^{m} (r_{i,k} \wedge r_{j,k})}{\sum_{k=1}^{m} (r_{i,k} \vee r_{j,k})}; \quad YXP(y_{i}, y_{j}) = \frac{\sum_{k=1}^{n} (r_{k,i} \wedge r_{k,j})}{\sum_{k=1}^{n} (r_{k,i} \vee r_{k,j})}$$

Luis Rocha 2002



## **Document and Keyword Proximity**

Typical IR Example: Knowledge Implied by Keywords

Given a binary relation A between sets of keywords K and documents D we extract two proximity relations:  $KDP(k_i, k_j)$  is the probability that both keywords  $k_i$  and  $k_j$  co-occur in the same document  $d \in D$ . Conversely,  $DKP(y_i, y_j)$  is the probability that both documents  $d_i$  and  $d_i$  contain the same keyword  $k \in K$ .

$$kdp(k_{i},k_{j}) = \frac{\sum_{k=1}^{m} (a_{i,k} \wedge a_{j,k})}{\sum_{k=1}^{m} (a_{i,k} \vee a_{j,k})} = \frac{N_{\cap}(k_{i},k_{j})}{N_{\cup}(k_{i},k_{j})} \quad dkp(k_{i},k_{j}) = \frac{\sum_{k=1}^{m} (a_{i,k} \wedge a_{j,k})}{\sum_{k=1}^{m} (a_{i,k} \vee a_{j,k})} = \frac{N_{\cap}(d_{i},d_{j})}{N_{\cup}(d_{i},d_{j})}$$

(Keyword Document Proximity)

(Document Keyword Proximity)







### **Pointwise Mutual Information**

Other non-proximity Probability Measures of Association

### **Conditional Probability**

Given a binary relation *R* between sets *X* and *Y* we extract :

$$P_{X}(x_{i}, x_{j}) = P(x_{i} | x_{j}) = \frac{\sum_{k=1}^{m} (r_{i,k} \wedge r_{j,k})}{\sum_{k=1}^{m} (r_{j,k})}; \quad P_{Y}(y_{i}, y_{j}) = P(y_{i} | y_{j}) = \frac{\sum_{k=1}^{n} (r_{k,i} \wedge r_{k,j})}{\sum_{k=1}^{n} (r_{k,j})}$$

 $P_X(x_i, x_j)$  is the probability that  $x_i$  is related in R to  $y \in Y$ , given that  $x_j$  is related to y.

 $P_Y(y_i, y_j)$  is the probability that  $y_i$  is related in R to  $x \in X$ , given that  $x_y$  is related to x.





# **Proximity vs. Conditional Probability**

$$XYP(x_{i}, x_{j}) = \frac{1}{\frac{1}{P_{X}(x_{j}, x_{i})} + \frac{1}{P_{X}(x_{i}, x_{j})} - 1}; \quad YXP(y_{i}, y_{j}) = \frac{1}{\frac{1}{P_{Y}(y_{j}, y_{i})} + \frac{1}{P_{Y}(y_{i}, y_{j})} - 1}$$

- $\blacksquare$   $P_X$  and  $P_Y$  are not symmetric
  - can measure a strong degree of association between two elements, when that association is one-sided only.
  - ► In many applications, when we think of a strong association between two elements, we expect both directions of association to be similar.
  - Distances are symmetric, proximity is the semantic inverse of distance.

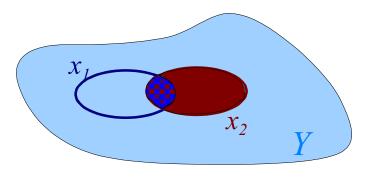


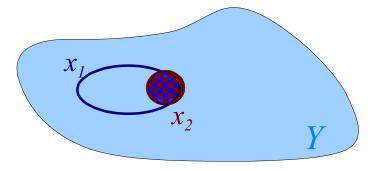




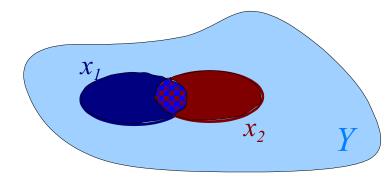
# **Conditional Probability and Proximity Measures**

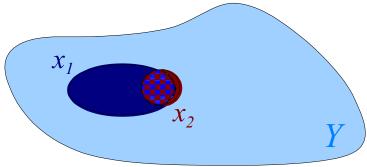
### **Conditional Probability**





### **Proximity**





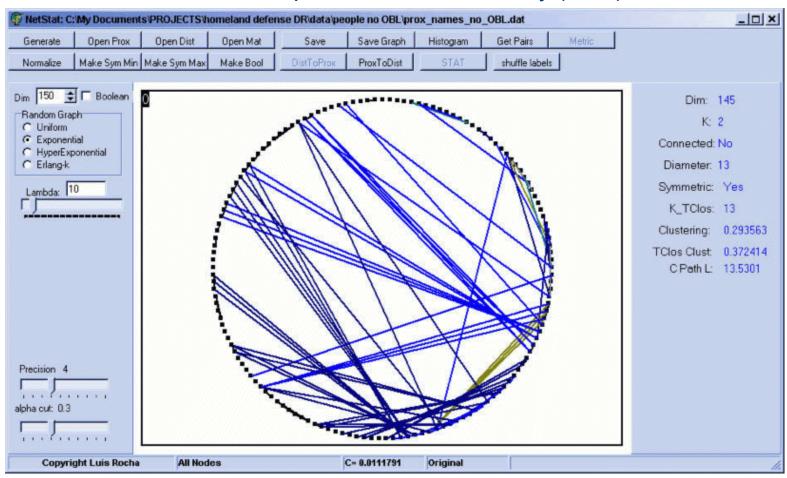
Luis Rocha 2002





# **Social Proximity Networks**

Terrorist Associations: People Document Proximity (PDP)

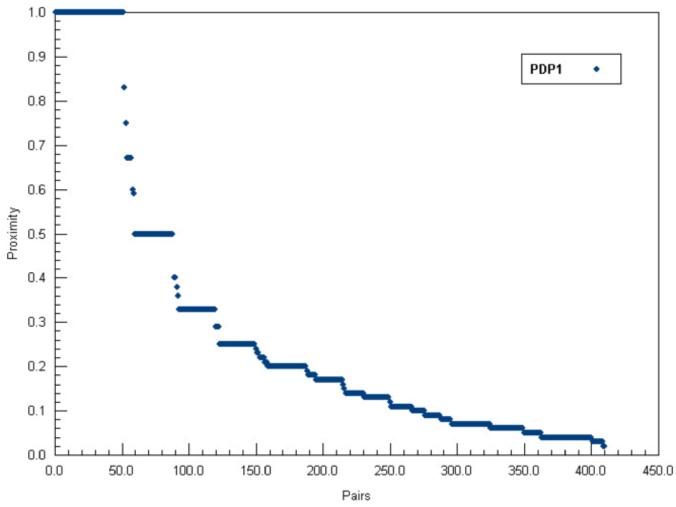






# **Proximity Distribution**

### PDP: exponential distribution



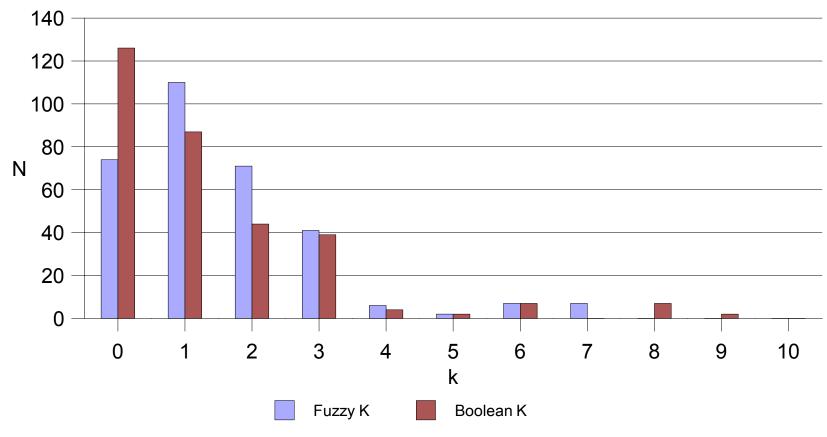
Luis Rocha 2002





# **PDP Histogram fo Node Degree**

### 318 People Names

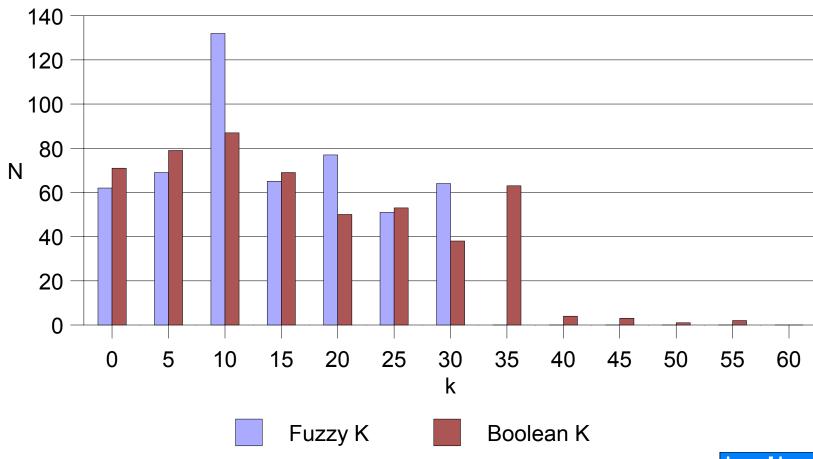


Luis Rocha 2002



# **IPP Histogram of Node Degree**

#### **520 ISSN**



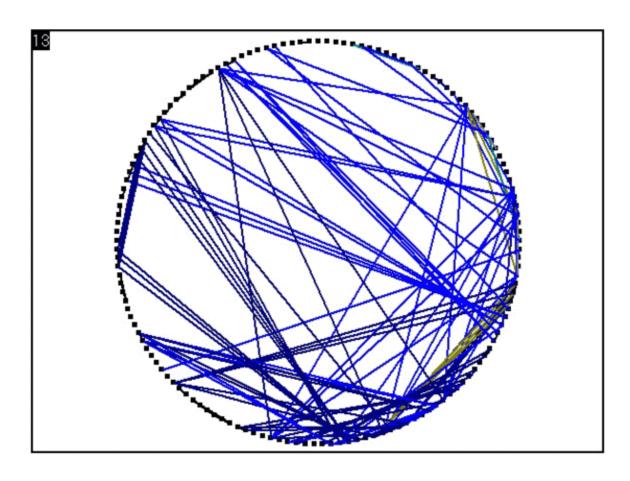
Luis Rocha 2002





# **Terrorist Networks**

#### PDP: transitive Closure







### **Terrorist Networks**

#### Highly Associated People in Documents

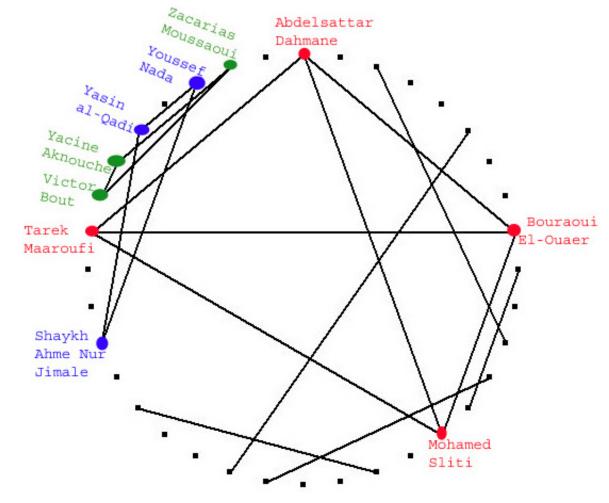






# **People Network**

#### Detail



Luis Rocha 2002





# **Using Information Retrieval**

#### Immunology Testcase

#### Cytokines Receptor Molecules IL-2 OR interleukin-2= CD25 OR tac. IL-3 OR interleukin-3 **>** CD122 IL-4 OR interleukin-4 CD132 OR "common gamma chain" IL-6 OR interleukin-6 ➤ CD123 IL- 7 OR interleukin-7 beta IL-8 OR interleukin-8 **►**CD124 IL-10 OR interleukin-10 CD126 IL-12 OR interleukin- 12 **CD130 OR gp130** IL-13 OR interleukin-13 **CD127** IL-15 OR interleukin-15 CXCR1 OR Cdw128a GM-CSF < CXCR2 OR Cdw128b **IFNgamma TNFalpha →**CD212 MCP-1 **▲**CD213a1 **△**CD213a2 Signaling molecules: CD116 their levels affect CD119 response ➤ CD120a ▲CD120b CCR2b

Luis Rocha 2002



### **Pointwise Mutual Information**

#### Information Retrieval

Turney, P.D. (2001). "Mining the Web for Synonyms: PMI-IR versus LSA on TOEFL." *Proceedings of the Twelfth European Conference on Machine Learning* (ECML-2001), Freiburg, Germany, pp. 491-502. <a href="http://extractor.iit.nrc.ca/reports/ECML2001.html">http://extractor.iit.nrc.ca/reports/ECML2001.html</a>

### PMI-IR developed to deal with Synonyms

- Problem word and set of choice words for synonyms (on TOEFL and ESL)
  - Problem: levied
  - Choices: imposed, believed, requested, correlated
- ▶ Assigns a *co-occurrence* score to each choice, and selects the choice that maximizes the score.
  - $score(choice_i) = p(problem | choice_i) = p(problem AND choice_i) / p(choice_i)$
  - In PMI-IR, the probabilities are calculated using IR from such sources as Altavista.







### **PMI-IR**

#### 4 Scores using Altavista

1. Conditional Probability with Altavista AND (when both terms appear in the same document)

$$score_1(choice_i) = \frac{hits(problem AND choice_i)}{hits(choice_i)}$$

2. Conditional probability with Altavista NEAR (when both terms appear within 10 words of each other in the same document)

$$score_2(choice_i) = \frac{hits(problem NEAR choice_i)}{hits(choice_i)}$$

3. Tends to reduce equal scores for synonyms and antonyms

$$score_{3}(choice_{i}) = \frac{hits(problem \, \text{NEAR} \, choice_{i}) \, \text{AND} \, \, \text{NOT}\big((problem \, \text{OR} \, choice_{i}) \, \text{NEAR} \, \text{"not"}\big)}{hits(choice_{i} \, \text{AND} \, \, \text{NOT}\big(choice_{i} \, \, \text{NEAR} \, \text{"not"}\big)\big)}$$

#### 4. Accounts for context words

LSA Problems: "Every year in the early spring farmers [tap] maple syrup from their trees (drain; boil; knock; rap)." The problem word *tap*, out of context, might seem to best match the choice words *knock* or *rap*, but the context maple syrup makes *drain* a better match for tap.





# **Proximity Queries**

$$prox_{1} (problem, choice_{i}) = \frac{hits(problem \text{ AND } choice_{i})}{hits(problem \text{ OR } choice_{i})}$$

$$prox_{2}(problem, choice_{i}) = \frac{hits(problem \text{ NEAR } choice_{i})}{hits(problem \text{ OR } choice_{i})}$$

### **NEAR**: co-occurrence within 10 words

$$prox_{3}(problem, choice_{i}) = \frac{hits((problem NEAR choice_{i}) NEAR context)}{hits(problem OR choice_{i})}$$

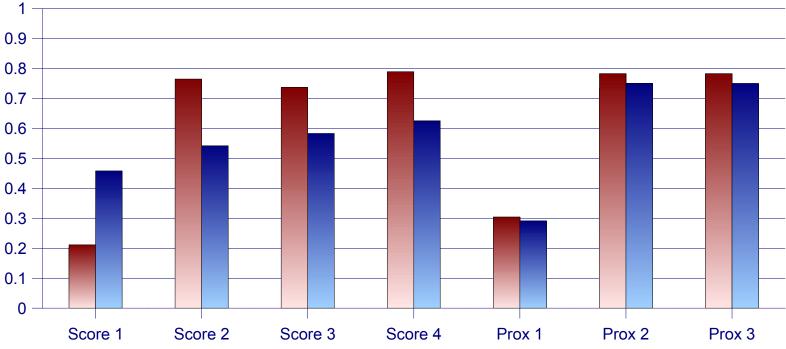
$$context = \{receptor\}$$





### **Precision and Recall**

#### Values Obtained with FaCSO



**Precision**: probability that an identified association is relevant

**Recall**: probability that an association has been identified given that it is relevant

http://www.c3.lanl.gov/~rocha

$$precision = \frac{\left\| \left\{ relevant \right\} \cap \left\{ retrieved \right\} \right\|}{\left\| \left\{ retrieved \right\} \right\|}$$

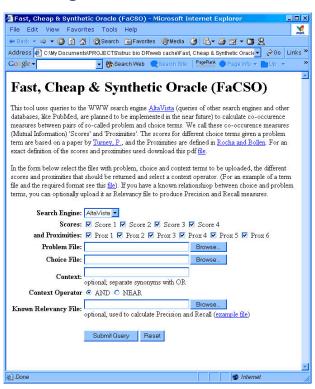
$$recall = \frac{\left\| \left\{ retrieved \right\} \cap \left\{ relevant \right\} \right\|}{\left\| \left\{ relevant \right\} \right\|}$$





## **Measuring Associations**

#### **Using Altavista**



- Discovers Relevant Associations
- Retrieves Documents substantiating the associations
- Being Developed for PubMed

# Fast, Cheap & Synthetic Oracle (FaCSO)

http://bimmer.c3.lanl.gov/~andreas/easyfast8.html

Luis Rocha 2002

Cytokine Set



rocha@lanl.gov

Luis Rocha

2002

eigenexpression

#### expression is increased (decreased) after infection with

SVD of Time-Dependent Expression Data

Eigengene 1

Eigengene 1: Increase in

infection

expression after

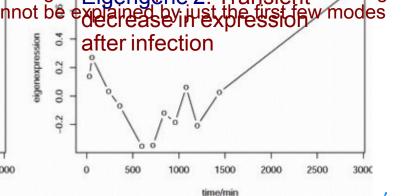
2500

Genes whose expression is positively (negatively)

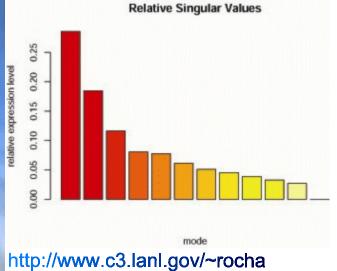
Gene expression (13000 genes) after already with with with with the company of th

expression is transiently decreased (increased) after infection with Herpes virus.

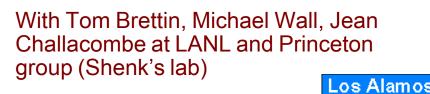
The singula Evaluación de explained by illet the first few modes



12 point time series (30min - 48hrs)



 $X = USV^{\mathrm{T}}$ 



Eigengene

Eigengene

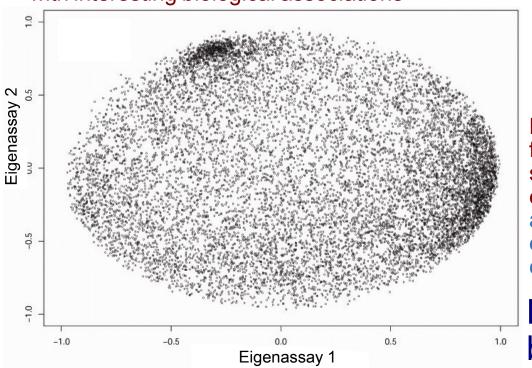
National Laboratory

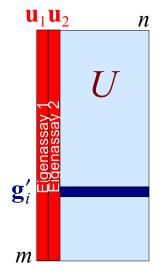


# **Biological Discovery via SVD**

**Eigenassay Coefficient Plot** 

LANL group found a second expression mode with interesting biological associations





Princeton group (Shenk's lab) found ~1200 genes that showed significant changes in expression at least 3 fold change in expression at at least 2 consecutive time points

How to help biologists discover function?

Luis Rocha 2002

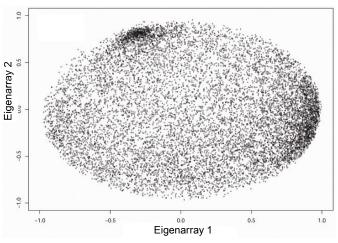




### **Automatic Functional Annotation**

Extract

#### Of Gene Clusters



Count number of times each gene <u>in</u> <u>a target group</u> is associated with a heading

Count number of times each gene *in HUGO* is associated with a heading

Statistical measure to see if a heading is mentioned by an unusually large number of genes in target group (given how many HUGO genes mention them)

Sets of genes most correlated and anti-correlated with each eigenarray (or cluster)

Checked likelihood that they are gene symbols (whether or not they cooccur with words like DNA, gene, etc.)

Genbank IDs Gene symbols

Collaboration with **Lada Adamic**, **Eytan Adair**, and **Bernardo Huberman** at *HP Labs*, Palo Alto.

Luis Rocha 2002



MeSH Heading	Sig	genes	ocurrence in target	Occurrence in HUGO
Aspergillosis, Allergic Bronchopulmonary	6.21	CCR2CR1HLAA	3	42
Immune Complex Diseases	4.56	CD48CCR2CR1HLAA	4	118
Leukemia, Lymphocytic, Acute, L2	4.29	CR1FHITHLAAXRCC4	4	129
Sequence Tagged Sites	4.17	CCR2DAXXEVI2AFHITGHRHRHLAAK	13	924
Leukemia, Myeloid, Chronic-Phase	4.15		3	82 90
Adenocarcinoma, Bronchiolo-Alveolar		FHITHLAAMUC5B	3	90
Ethers	3.88		4	149 404
Antibodies, Blocking		CD48CCR2CR1GHRHRHLAAMCAMC	7	404
Leishmaniasis		CR1HLAATNP1	3	102
Fructose-Bisphosphatase		CCR2FBP2GIT2	3	103
Bone Marrow Purging		CD48CR1HLAA	3	110
Rhinitis		CD48CR1MUC5B	3	112
Agglutinins		CR1HLAAMUC5B	3	112
Homosexuality	3.25	CCR2CR1HLAA	3	117
Linkage (Genetics)		AMPD3CAMK2ARUNX2CD48CHRNA3(	30	3753
Neural Tube Defects		CD48GLI3HLAAFBP2	4	194 196
Carcinoid Tumor	3.16	FHITGHRHRHLAAMUC5B	4	196
Hispanic Americans	3.11	CCR2CR1HLAA	3	124
Polymorphism, Restriction Fragment Lengtl		CAMK2ACCR2CR1EVI2AFHITGHRHR-		2355
Communicable Diseases		CD48CR1HLAA	3	125 127
AIDS Vaccines		CCR2CR1HLAA	3	127
Gene Order		HLAATNP1SNX3	3	127
Tuberculosis	3.04		5	293 128
Hemoglobinuria, Paroxysmal		CD48CR1HLAA	3	128
Lupus Nephritis	3.02	CD48CCR2CR1HLAA	4	207 131
Hirschsprung Disease		EDN3GLI3HLAA	3	131
Belgium		CCR2CR1HLAA	3	The state of the s
Protein Isoforms		ABCA2RUNX2CD48CCR2CR1GHRHR-		2298
Haplotypes	2.88	CD48CCR2CR1EDN3EVI2AGHRHRH	16	1700



# **MeSH Headings**

### Correlated with Second Eigenassay

Genes involved in transcription regulation, immune response, oncogenesis as well as growth factors/cytokines and their receptors

MeSH Heading	Sig	genes	ocurrence in target	Occurrence in HUGO
Aspergillosis, Allergic Bronchopulmonary		CCR2CR1HLAA	3	42
Immune Complex Diseases		CD48CCR2CR1HLAA	4	118
Leukemia, Lymphocytic, Acute, L2	4.29	CR1FHITHLAAXRCC4	4	129
Sequence Tagged Sites	4.17	CCR2DAXXEVI2AFHITGHRHRHLAAK	13	924
Leukemia, Myeloid, Chronic-Phase	4.15		3	82
Adenocarcinoma, Bronchiolo-Alveolar		FHITHLAAMUC5B	3	90
Ethers		CD48CR1HLAALY6E	4	149
Antibodies, Blocking		CD48CCR2CR1GHRHRHLAAMCAMC	7	404
Leishmaniasis		CR1HLAATNP1	3	102
Fructose-Bisphosphatase	3.56	CCR2FBP2GIT2	3	103
Bone Marrow Purging	3.4		3	110
Rhinitis		CD48CR1MUC5B	3	112
Agglutinins		CR1HLAAMUC5B	3	112
Homosexuality		CCR2CR1HLAA	3	117
Linkage (Genetics)		AMPD3CAMK2ARUNX2CD48CHRNA30	30	3753
Neural Tube Defects	3.18		4	194
Carcinoid Tumor		FHITGHRHRHLAAMUC5B	4	196
Hispanic Americans	3.11		3	124
Polymorphism, Restriction Fragment Lengt		CAMK2ACCR2CR1EVI2AFHITGHRHR-	21	2355
Communicable Diseases		CD48CR1HLAA	3	125
AIDS Vaccines		CCR2CR1HLAA	3	127
Gene Order	3.06	HLAATNP1SNX3	3	127
Tuberculosis	3.04		5	293
Hemoglobinuria, Paroxysmal	3.04		3	128
Lupus Nephritis		CD48CCR2CR1HLAA	4	207
Hirschsprung Disease		EDN3GLI3HLAA	3	131
Belgium	2.93	CCR2CR1HLAA	3	134
Protein Isoforms	2.9	ABCA2RUNX2CD48CCR2CR1GHRHR-	20	2298
Haplotypes	2.88	CD48CCR2CR1EDN3EVI2AGHRHRHI	16	1700



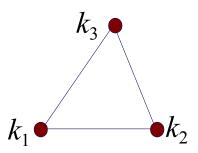


# **Distance from Proximity**

#### Semi-metric Behavior

$$kdp(k_{i},k_{j}) = \frac{\sum_{k=1}^{m} (a_{i,k} \wedge a_{j,k})}{\sum_{k=1}^{m} (a_{i,k} \vee a_{j,k})} = \frac{N_{\cap}(k_{i},k_{j})}{N_{\cup}(k_{i},k_{j})}$$

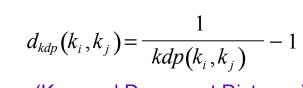
(Keyword Document Proximity)



$$d(k_1, k_2) \le d(k_1, k_3) + d(k_3, k_2)$$
Metric
 $d(k_1, k_2) > d(k_1, k_3) + d(k_3, k_2)$ 

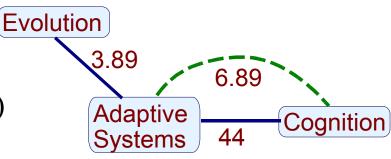
Semi-metric

http://www.c3.lanl.gov/~rocha



(Keyword Document Distance)

d is a distance function because it is a nonnegative, symmetric, realvalued function such that d(k, k) = 0



Semi-metric ratio: 6.3861

Los Alamos National Laboratory



# **Distance from Proximity**

#### Generic Case

$$XYP(x_{i}, x_{j}) = \frac{\sum_{k=1}^{m} (r_{i,k} \wedge r_{j,k})}{\sum_{k=1}^{m} (r_{i,k} \vee r_{j,k})}; \quad YXP(y_{i}, y_{j}) = \frac{\sum_{k=1}^{n} (r_{k,i} \wedge r_{k,j})}{\sum_{k=1}^{n} (r_{k,i} \vee r_{k,j})}$$

$$d_X(x_i, x_j) = \frac{1}{XYP(x_i, x_j)} - 1; \quad d_Y(y_i, y_j) = \frac{1}{YXP(y_i, y_j)} - 1$$

Distance from a Proximity Graph is semi-Metric Distance from a Similarity Graph is Metric

Luis Rocha 2002



# **Measuring Semi-Metric Behavior**

#### Semi-metric Measures

### Semi-metric ratio

Absolute measure of indirect distance reduction

$$s(x_i, x_j) = \frac{d_{direct}(x_i, x_j)}{d_{shortest}(x_i, x_j)}$$

#### Relative Semi-metric ratio

► Distance reduction against maximum contraction

$$rs(x_i, x_j) = \frac{d_{direct}(x_i, x_j) - d_{shortest}(x_i, x_j)}{d_{max} - d_{min}}$$

### Below Average Ratio

► Captures semi-metric distance reductions which contract to below the average distance for a given node. Captures some of the cases of initial ∞ distance

$$b(x_i, x_j) = \frac{\overline{d_{x_i}}}{d_{shortest}(x_i, x_j)}$$





### 86 Keywords



### **Dissertation Database**

ADAPTIVE SYSTEMS	COGNITION	Semi-metric Ratio	6.3861 Relative Semi-metric	0.8434	1
EVOLUTION	CONSTRUCTIVISM	Semi-metric Ratio	5.0000 Relative Semi-metric	0.7636	2
EVOLUTION	PSYCHOLOGY	Semi-metric Ratio	5.0000 Relative Semi-metric	0.7273	3
EVOLUTION	DNA	Semi-metric Ratio	4.6936 Relative Semi-metric	0.6439	4
LIFE	COGNITION	Semi-metric Ratio	4.5455 Relative Semi-metric	0.6559	5
EVOLUTION	CONTROL	Semi-metric Ratio	4.5407 Relative Semi-metric	0.7620	6
MATHEMATICS	SYSTEMS THEORY	Semi-metric Ratio	4.4205 Relative Semi-metric	0.6507	7
CYBERNETICS	THEORETICAL BIOLOGY	Semi-metric Ratio	4.3593 Relative Semi-metric	0.5780	8
ARTIFICIAL LIFE	NEURAL NETWORKS	Semi-metric Ratio	4.2918 Relative Semi-metric	0.3486	9
ARTIFICIAL INTELLIGENCE	SELF-ORGANIZING SYSTEMS	Semi-metric Ratio	4.0897 Relative Semi-metric	0.5323	10
ROBOTICS	COGNITION	Semi-metric Ratio	3.9759 Relative Semi-metric	0.5614	11
MATHEMATICS	MEMORY	Semi-metric Ratio	3.8509 Relative Semi-metric	0.5216	12
ROBOTICS	MATHEMATICS	Semi-metric Ratio	3.8028 Relative Semi-metric	0.4523	13
LIFE	PHILOSOPHY	Semi-metric Ratio	3.7928 Relative Semi-metric	0.6861	14
ROBOTICS	PHILOSOPHY	Semi-metric Ratio	3.7525 Relative Semi-metric	0.6168	15
PHILOSOPHY	EMERGENCE	Semi-metric Ratio	3.7365 Relative Semi-metric	0.6325	16
COGNITION	SEMIOTICS	Semi-metric Ratio	3.7353 Relative Semi-metric	0.5825	17
EVOLUTION	MOLECULAR BIOLOGY	Semi-metric Ratio	3.7229 Relative Semi-metric	0.5984	18
EVOLUTION	CELLULAR AUTOMATA	Semi-metric Ratio	3.7218 Relative Semi-metric	0.6316	19
EVOLUTION	INFORMATION THEORY	Semi-metric Ratio	3.7037 Relative Semi-metric	0.7134	20

9% Semi-metric 25% below Average

C	COMPUTER NETWORKS	STATE-SPACE METHODS	Under Average	7.5000
Λ	MORPHOLOGY	GROWTH	<b>Under Average</b>	5.3000
C	COMPUTER GRAPHICS	FORM	<b>Under Average</b>	4.7037
Λ	MORPHOLOGY	FORM	<b>Under Average</b>	4.2400
Λ	MORPHOLOGY	PALEONTOLOGY	Under Average	3.5333
Λ	MORPHOLOGY	CONTINGENCY	<b>Under Average</b>	3.5333
F	ROBOTICS	NEURAL NETWORKS	Under Average	3.3420
E	VOLUTION	NEURAL NETWORKS	Under Average	3.1134
E	VOLUTION	DNA	Under Average	3.0404
C	COGNITION	THEORETICAL BIOLOGY	Under Average	3.0377

Luis Rocha 2002



# **Trends in Collections**

### **ARP Database**

leukemia	myocardi	Semi-metric Ratio	272.1996 Relative Semi-metric	0.4981	1
hormon	thin	Semi-metric Ratio	214.0797 Relative Semi-metric	0.9953	2
care	excit	Semi-metric Ratio	213.5900 Relative Semi-metric	0.9953	3
gene	equat	Semi-metric Ratio	205.7649 Relative Semi-metric	0.9951	4
film	transcript	Semi-metric Ratio	204.5103 Relative Semi-metric	0.9951	5
spectroscopi	care	Semi-metric Ratio	194.3478 Relative Semi-metric	0.9949	6
transcript	thin	Semi-metric Ratio	193.0644 Relative Semi-metric	0.9948	7
pressur	t-cell	Semi-metric Ratio	190.8173 Relative Semi-metric	0.9948	8
film	mutat	Semi-metric Ratio	186.8350 Relative Semi-metric	0.9946	9
vascular	catalyst	Semi-metric Ratio	185.3671 Relative Semi-metric	0.9946	10
film	endoth	Semi-metric Ratio	183.0219 Relative Semi-metric	0.9945	11
film	macrophag	Semi-metric Ratio	180.4128 Relative Semi-metric	0.9945	12
nonlinear	nerv	Semi-metric Ratio	177.6419 Relative Semi-metric	0.9944	13
film	clone	Semi-metric Ratio	175.6775 Relative Semi-metric	0.9943	14
mutat	equat	Semi-metric Ratio	175.1138 Relative Semi-metric	0.9943	15
film	secretion	Semi-metric Ratio	174.9438 Relative Semi-metric	0.9943	16
thin	endoth	Semi-metric Ratio	173.8007 Relative Semi-metric	0.9942	17
pressur	leukemia	Semi-metric Ratio	172.2365 Relative Semi-metric	0.9942	18
thin	macrophag	Semi-metric Ratio	171.4462 Relative Semi-metric	0.9942	19
film	mortal	Semi-metric Ratio	169.9975 Relative Semi-metric	0.9941	20
clone	thin	Semi-metric Ratio	167.1643 Relative Semi-metric	0.9940	21

95% Semi-metric 35% Below Average

Luis Rocha 2002

leukemia	myocardi	Under Average	77.7665
thin	nitric	Under Average	50.5213
equat	messenger-rna	Under Average	42.3600
chemotherapi	myocardi	Under Average	41.6956
nonlinear	nerv	Under Average	40.1634
film	risk	Under Average	40.0989
equat	transcript	Under Average	39.9494
equat	clone	Under Average	39.9156
film	hormon	Under Average	39.6987
equat	gene-express	Under Average	37.0435





### **Analysing Different Document Networks**

#### For Semi-Metric Behavior

#### PCP Web

- ► Collection of dictionary-like definitions about Systems Research topics; each of these 423 web pages is associated with a specific concept (e.g. "Adaptive Systems").
  - Proximity Data extracted from hyperlink structure (Symmetric)
  - Adapted Hyperlink Structure from user paths extracted from web logs using Bollen's Algorithms (Symmetric)

#### ISSN

▶ Network of 472 Research Journal Titles (e.g. "Communications of the ACM" and "BioSystems"), identified by their ISSN. Adapted using the same methodology used for the adapted PCP web site data (symmetric).

#### Word Norm

▶ Nelson et al' s associative graphs between pairs of words from free association experiments with more than 6000 subjects; weights characterize the semantic proximity between words as understood by the population of subjects. We used a subset of 150 words from this dataset (of about 5000 words): the 150 most common English nouns, (words such as "art", "car", "face").

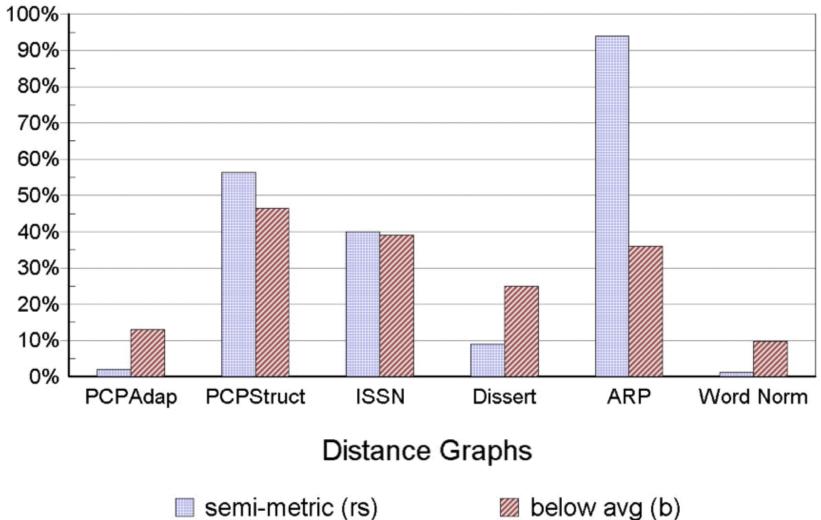
#### Random Distance Graphs

► Uniform, Exponential, Hyperexponential Proximity Distributions





# Percentage of Semi-metric Pairs

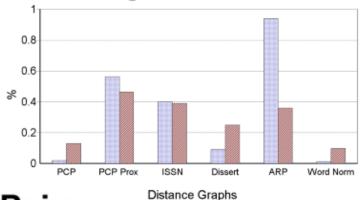


Luis Rocha 2002





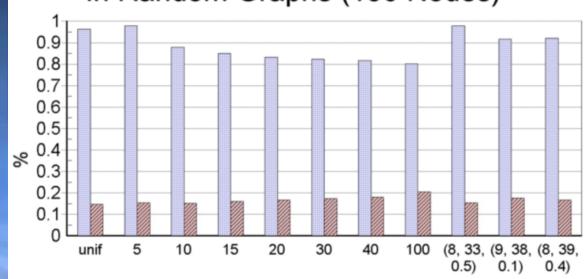
#### Percentage of Semi-metric Pairs



semi-metric (rs) 💹 below avg (b)

# Percentage of Semi-metric Pairs

In Random Graphs (150 Nodes)



**Distance Graphs** 

semi-metric (rs) http://www.c3.lanl.gov/~rocha

below avg (b)



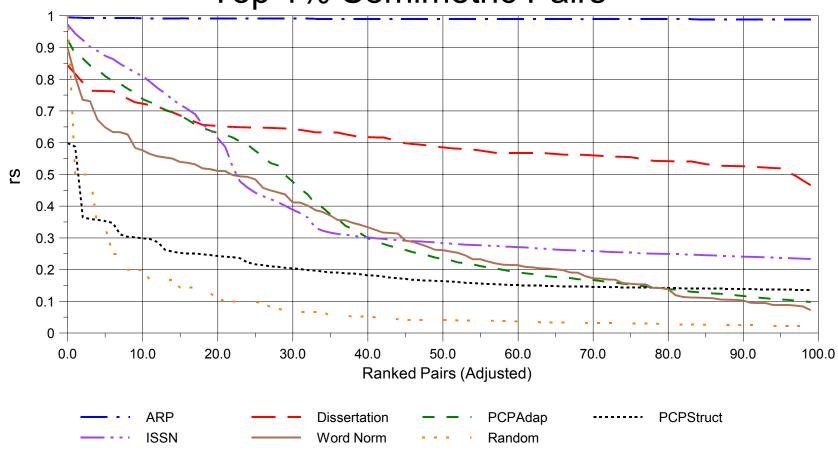
Luis Rocha

2002



# TRS<sup>1%</sup>

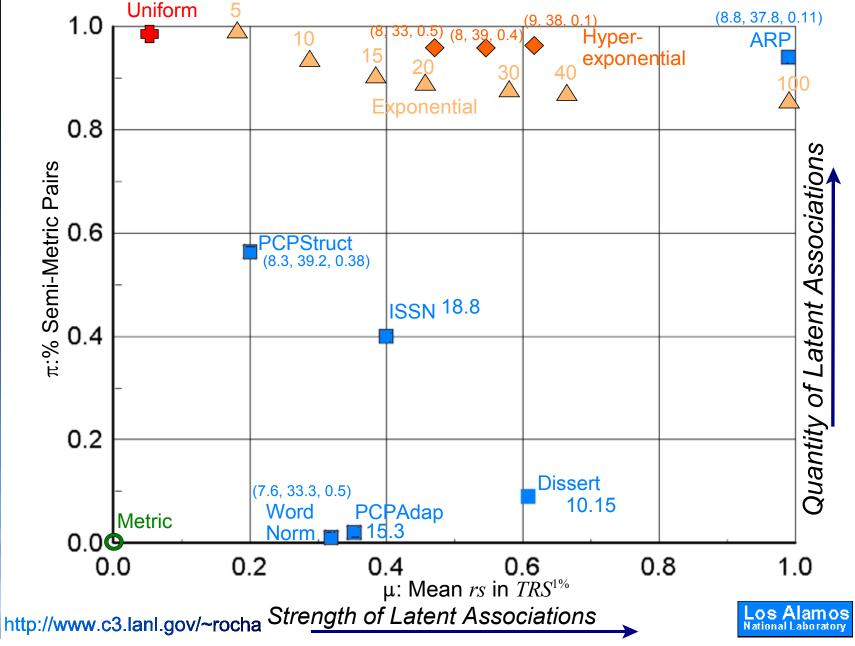
# Top 1% Semimetric Pairs



Luis Rocha 2002



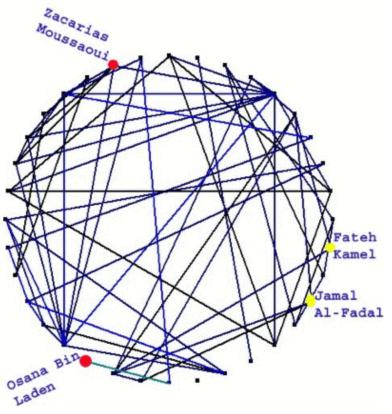
Luis Rocha





### **Identification of Latent Associations**

#### **Terrorist Network Example**



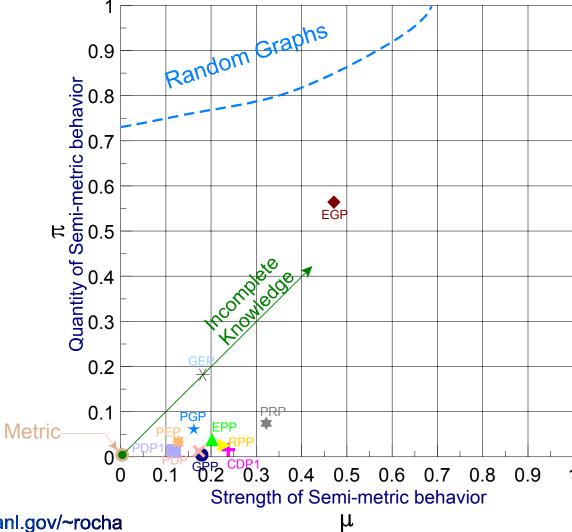
- Pairs with larger semi-metric behavior denote a latent association
  - Not grounded on direct evidence provided by the relation R, but rather implied by the overall network of associations in this relation.
  - Meaning depends on the semantics of the application
    - In graphs of keyword co-occurrence in documents: associated with novelty and can be used to identify trends.
    - In terrorist networks it may identify pairs of people, groups, etc. for which we do not have direct evidence, in the available documents, that a real association exists, but who could easily be indirectly associated
  - In recommendation system for journals now at LANL

Luis Rocha 2002



### Does a latent association imply missing evidence?

#### Incomplete Knowledge



Luis Rocha 2002

http://www.c3.lanl.gov/~rocha



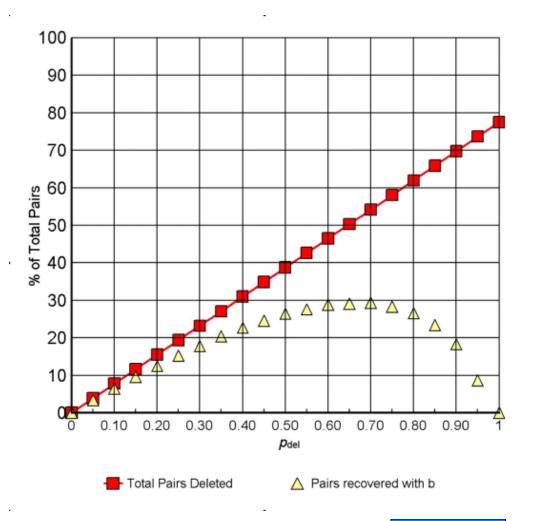
# **Detecting Incomplete Knowledge**

#### Random Deletion Experiments.

### Perfect Knowledge

- Transitive Closure of real graph
- Metric Distance Graph
- Incomplete Knowledge
  - ► Each positive association is deleted with probability *p*<sub>del</sub>
  - ► 100 graphs for each value of p<sub>del</sub>

### **Full Deletion**

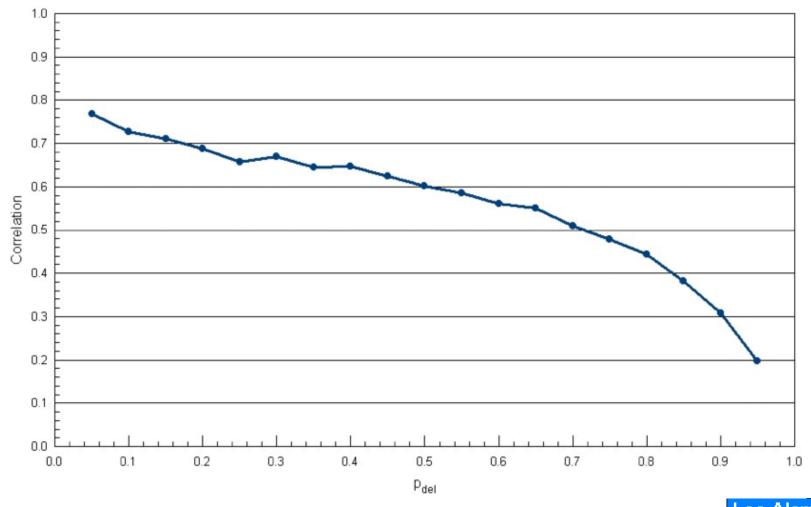


Luis Rocha 2002



### **Full Deletion**

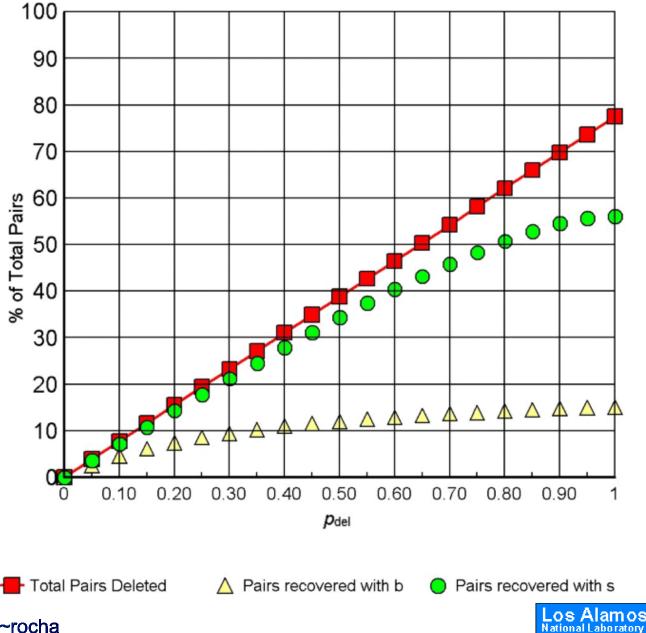
#### Correlation of value of b with deleted value



Luis Rocha 2002



# Partial Deletion

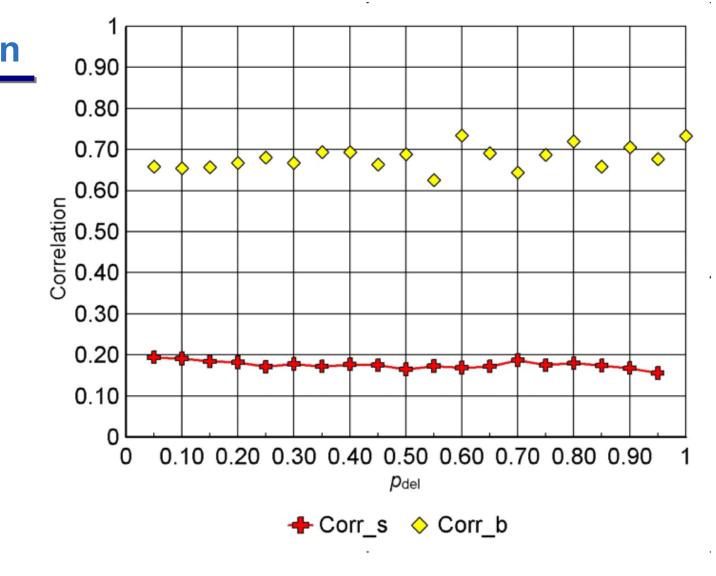


Luis Rocha 2002



# Partial Deletion

Parameter Correlation



Luis Rocha 2002



# **Proximity 6**

 $prox_{6}(problem, choice_{i}) = \frac{hits((problem NEAR choice_{i}) NEAR context)}{hits(problem OR choice_{i})}$ 

#### Semi-metric Associatons

### Cytokines: Problem Terms

Receptor Molecules: choice terms

Existing cooccurrence IL-15, CD122 IL-2, CD130 IL-7, CD126 IL-4, CD122 IL-13, CD132 IL-10, CD130

Null cooccurrence IL-7, CD122 IL-15, CD123 IL-15, CD127 TNFalpha, CD120a IL-15, CD124 IL-7, CD123 IL-15, CD120a

Luis Rocha 2002

